

*In the Specification*

Please amend the paragraph at lines 7-26 of page 44 as follows:

A variety of data storage structures are available to a skilled artisan for creating a computer readable medium having recorded thereon the atomic structure coordinates of the invention or portions thereof and/or X-ray diffraction data. The choice of the data storage structure will generally be based on the means chosen to access the stored information. In addition, a variety of data processor programs and formats can be used to store the sequence and X-ray data information on a computer readable medium. Such formats include, but are not limited to, LuxS Data Bank ("PDB") format (Research Collaboratory for Structural Bioinformatics; World Wide Web address: [rcsb.org/pdb/docs/format/pdbguide2.2/guide2.2\\_frame.html](http://www.rcsb.org/pdb/docs/format/pdbguide2.2/guide2.2_frame.html)); [http://www.resb.org/pdb/docs/format/pdbguide2.2/guide2.2\\_frame.html](http://www.resb.org/pdb/docs/format/pdbguide2.2/guide2.2_frame.html)); Cambridge Crystallographic Data Centre format (World Wide Web address: [ccdc.cam.ac.uk/support/csd\\_doc/volume3/z323.html](http://www.ccdc.cam.ac.uk/support/csd_doc/volume3/z323.html)) [http://www.ccdc.cam.ac.uk/support/csd\\_doc/volume3/z323.html](http://www.ccdc.cam.ac.uk/support/csd_doc/volume3/z323.html)); Structure-data ("SD") file format (MDL Information Systems, Inc.; Dalby *et al.*, 1992, J. Chem. Inf. Comp. Sci. 32:244-255), and line-notation, *e.g.*, as used in SMILES (Weininger, 1988, J. Chem. Inf. Comp. Sci. 28:31-36). Methods of converting between various formats read by different computer software will be readily apparent to those of skill in the art, *e.g.*, BABEL (v. 1.06, Walters & Stahl, ©1992, 1993, 1994; World Wide Web Address: [brunel.ac.uk/departments/chem./babel.htm](http://www.brunel.ac.uk/departments/chem./babel.htm).) <http://www.brunel.ac.uk/departments/chem./babel.htm>.) All format representations of the polypeptide coordinates described herein, or portions thereof, are contemplated by the present invention. By providing computer readable medium having stored thereon the atomic coordinates of the invention, one of skill in the art can routinely access the atomic coordinates of the invention, or portions thereof, and related information for use in modeling and design programs, described in detail below.